

Dynamic Spin Response for Heisenberg Ladders

J. Piekarewicz

*Supercomputer Computations Research Institute,
Florida State University, Tallahassee, FL 32306*

J.R. Shepard

*Department of Physics,
University of Colorado, Boulder, CO 80309
(February 1, 2008)*

Abstract

We employ the recently proposed plaquette basis to investigate static and dynamic properties of isotropic 2-leg Heisenberg spin ladders. Simple non-interacting multi-plaquette states provide a remarkably accurate picture of the energy/site and dynamic spin response of these systems. Insights afforded by this simple picture suggest a very efficient truncation scheme for more precise calculations. When the small truncation errors are accounted for using recently developed Contractor Renormalization techniques, very accurate results requiring a small fraction of the computational effort of exact calculations are obtained. These methods allow us to determine the energy/site, gap, and spin response of 2×16 ladders. The former two values are in good agreement with density matrix renormalization group results. The spin response calculations show that nearly all the strength is concentrated in the lowest triplet level and that coherent many-body effects enhance the response/site by nearly a factor of 1.6 over that found for 2×2 systems.

PACS numbers: 75.10.Jm, 75.40.Gb, 75.40.Mg

Heisenberg spin ladders are deceptively simple systems consisting of n_c parallel spin chains (legs) connected by pairwise interactions (rungs). Topologically, ladders are intermediate to chains ($n_c \rightarrow 1$) and planes ($n_c \rightarrow \infty$) but, as is by now well-established, they possess physical properties which cannot be guessed on the basis of their behavior in the 1D and 2D limits. Perhaps the greatest surprise is the existence of a spin gap for even-leg antiferromagnetic spin-1/2 ladders; chains and planes are gapless as are odd-leg ladders [1]. Apart from their intrinsic interest as rich mathematical systems, spin ladders are currently the objects of intense scrutiny because of the possibility that they may afford insights into the dynamics of high temperature superconductors [1,2]. Such inquiries are enlivened by the fact that spin ladders appear to be realized in certain compounds, 2-leg ladders in the form of vanadyl pyrophosphate being perhaps the most prominent example [1,3]. During the past few years, consistent theoretical and experimental pictures of the static properties of spin ladders (*e.g.*, the energy/site and the gap) have emerged. On the theoretical side, a variety of numerical methods have been employed including direct diagonalization, Lanczos techniques, quantum Monte Carlo (QMC) [4] and density matrix renormalization group (DMRG) approaches [5]. Progress in understanding dynamical features—including spin-triplet dispersion relations and spin responses [4]—has been somewhat slower, in part because the most powerful methods for studying static quantities, such as QMC and DMRG, cannot straightforwardly provide dynamical information. Studies of dynamical properties have typically relied on a combination of brute-force diagonalization (aided by Lanczos) [4] and analytic (or semi-analytic) methods based on perturbation theory [4–7], the latter frequently being used qualitatively to illuminate the underlying physics of the former. In the present letter, we suggest that such studies are hindered by two shortcomings: (*i*) that numerical and analytic treatments usually employ different bases and (*ii*) that neither basis is ideally suited to isotropic 2-leg spin ladders. In a recent paper [8] we proposed an alternative basis—to which we refer as the “plaquette basis”—which is well-suited to both numerical and analytic treatments and which reveals the physical origin of many dynamical features in an especially clear fashion. In the present paper, we exploit the plaquette basis to compute static and dynamic properties of 2-leg ladders with up to 32 sites. The results of the full brute-force diagonalizations (which are of course independent of the basis) can be reproduced with remarkable accuracy by an almost trivial model of non-interacting plaquettes.

The conventional “ S_z ” basis is very simple to construct and has been used almost exclusively in direct diagonalization calculations. A basis state is simply the product of spin-up or spin-down wavefunctions at each site. Matrix elements are simple to evaluate but, as shown in Ref. [8,9], eigenvectors are very complicated. Analytic methods typically employ the “rung” or “singlet-triplet” basis in which the Hamiltonian is diagonal in the limit in which the coupling along the rungs (J_\perp) is much stronger than the coupling along the chains (J_\parallel) [4]. In this limit, the system consists of independent rungs, each of which can have overall spins of zero or one with eigenenergies of $-3/4 J_\perp$ and $+1/4 J_\perp$, respectively. The interaction proportional to J_\parallel is treated as a perturbation—which is problematic for the physically relevant [1] case of $J_\parallel \simeq J_\perp$. This basis has not been used in direct diagonalization calculations until very recently [9].

The plaquette basis [8] is more complicated to construct. The ladder is decomposed into distinct pairs of adjacent rungs. These 2×2 objects are the plaquettes. For the isotropic ($J_\parallel = J_\perp \equiv 1$) two-leg ladders studied here, the Hamiltonian is

$$H = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (1)$$

where the sum is over nearest-neighbor pairs. This Hamiltonian can be written as the sum of H_0 , which contains the intra-plaquette interactions, and V , which includes the interactions between plaquettes. The intra-plaquette Hamiltonian H_0 is expressible as

$$H_0 = \sum_i h_0^{(i)} ; \quad h_0^{(i)} = (\vec{S}_1^{(i)} + \vec{S}_4^{(i)}) \cdot (\vec{S}_2^{(i)} + \vec{S}_3^{(i)}) , \quad (2)$$

where i labels a specific plaquette. H_0 is diagonal in the plaquette basis:

$$H_0 |\Phi_{\text{plaq}}\rangle = E_{\text{plaq}} |\Phi_{\text{plaq}}\rangle , \quad (3)$$

where $|\Phi_{\text{plaq}}\rangle$ (E_{plaq}) is a direct product (sum) of single-plaquette wavefunctions (energies), each of the form [8]:

$$|\phi_\alpha\rangle = |(s_1 s_4)l_{14}, (s_2 s_3)l_{23}; jm\rangle , \quad (4)$$

$$\epsilon_\alpha = \frac{1}{2}[j(j+1) - \ell_{14}(\ell_{14}+1) - \ell_{23}(\ell_{23}+1)] . \quad (5)$$

In this basis the two *diagonal* pairs of spins are coupled to well-defined total angular momentum, ℓ_{14} and ℓ_{23} , which can equal zero or one. These two link angular momenta are in turn coupled to a total plaquette angular momentum j with projection m .

The single plaquette ground state has $\ell_{14} = \ell_{23} = 1$ and $j = 0$; the energy of this state is -2 . The next lowest (triply degenerate) state also has $\ell_{14} = \ell_{23} = 1$ but $j = 1$; its energy is -1 . The remaining states have energies greater than or equal to zero. Thus, the low-energy degrees of freedom for a single plaquette always have diagonal or link spins coupled to triplets and total plaquette angular momentum of zero or one. In this sense, as far as low-energy configurations are concerned, the intra-plaquette interactions “freeze out” all but triplet-triplet modes. These observations suggest that the low-energy spectrum of multi-plaquette systems will be relatively simple to describe in the plaquette basis where the relatively few “frozen” configurations—made up of only triplet-triplet single-plaquette states—should dominate. Examination of exact eigenstates determined by direct diagonalization confirms this speculation. For example, the singlet ground state of the 2×8 ladder is dominated by the one frozen configuration corresponding to the non-interacting ($V \rightarrow 0$) ground state (*i.e.*, four frozen $j = 0$ single-plaquette states). This particular configuration appears with an amplitude of 0.776. Moreover, four frozen configurations—out of a total of 1430 states in the basis—account for 82% of the total probability. We also note that simple non-interacting multi-plaquette states yield a surprisingly good estimate of the energy/site, namely, -0.5 , which compares reasonably well with the bulk value as determined by DMRG [5], namely, -0.57804 . Simple second order perturbation theory [9] improves the plaquette basis value to -0.55816 which corresponds to a 3.4% discrepancy. The price which must be paid for using the plaquette basis is that matrix elements are not simple to evaluate but can be handled with the sophisticated methods of Racah algebra used routinely in atomic and nuclear physics [10].

The dominance of frozen configurations suggests that a truncation which retains only these states should be quite accurate. As shown in Ref. [8], such is indeed the case. Energies

for low-lying states of 2×6 ladders computed using this truncated basis (to which we refer as the “frozen basis” in what follows) are within 5 to 10% of the exact values. As the frozen basis is much smaller than the full basis, its use results in a vast reduction of computational effort. As was also discussed in Ref. [8], it is possible to systematically correct for these small truncation errors by constructing an effective low-energy Hamiltonian to be used with the frozen basis. We accomplish this via the recently developed COnttractor REnormalization (CORE) method [11]. Here the effective Hamiltonian is expressed as a cluster expansion. In the CORE lexicon, truncations induce new “range- r ” interactions which depend on the quantum numbers of clusters containing r adjacent blocks; in our present treatment, these blocks are the plaquettes. In Ref. [8] we showed that, for 2×6 ladders, including range-2 CORE contributions for calculations of energies of low-lying states in the frozen basis brought discrepancies with exact results down to the level of 2% or less.

In the present work, we examine larger systems, the largest being a 2×16 ladder. Moreover, we include range-3 contributions to the effective Hamiltonian. At this order in the CORE treatment, the low-energy spectrum of the 2×6 ladder becomes exact by construction. The prediction for the ground state of the 2×8 ladder in the frozen basis at range-3 differs from the exact result by less than 0.02%; the discrepancy for the first excited state is even smaller. Our present calculations of the energy/site and the gap are summarized in Table I. We compare our range-3 results with either exact (for 2×8) or DMRG [12] (for 2×16) calculations. We also note that the CORE calculations for the 2×16 ladder require roughly the same computational effort as the exact calculations for the 2×8 system.

We now turn to the computation of dynamical quantities, focusing on the dynamical spin response,

$$S(\vec{q}, \omega) = \sum_n |\langle \Psi_n | \vec{S}(\vec{q}) | \Psi_0 \rangle|^2 \delta(\omega - \omega_n) , \quad (6)$$

where $|\Psi_0\rangle$ is the exact ground state of the system and $|\Psi_n\rangle$ is an excited state with excitation energy ω_n . Since the transition operator $\vec{S}(\vec{q})$ transforms as a rank-1 tensor (*i.e.*, a vector) the only excited states that can be reached from the singlet ground state have total angular momentum of one. The spin transition operator is

$$\vec{S}(\vec{q}) = \sum_i \vec{S}_i e^{i\vec{q} \cdot \vec{r}_i} , \quad (7)$$

where the sum is over all sites and \vec{q} is the momentum transfer to the ladder. $S(\vec{q}, \omega)$ can be measured, *e.g.*, by inelastic neutron scattering [13]. Of particular interest is the dynamic spin response probed at a momentum transfer (in units of the lattice spacing) of $\vec{q} \equiv \vec{q}_{\pi\pi} = (\pi, \pi)$. Clearly

$$\vec{S}(\vec{q}_{\pi\pi}) = \sum_i (-)^{\langle i \rangle} \vec{S}_i , \quad (8)$$

where $(-)^{\langle i \rangle}$ is a phase which flips in going from a site to any of its nearest neighbors. The essential properties of $S(\vec{q}_{\pi\pi}, \omega)$ are readily apparent in the plaquette basis. For a single 2×2 plaquette,

$$\vec{S}(\vec{q}_{\pi\pi}) \rightarrow (\vec{S}_1 + \vec{S}_4) - (\vec{S}_2 + \vec{S}_3) = \vec{L}_{14} - \vec{L}_{23} . \quad (9)$$

We see immediately that this operator *cannot* break the frozen triplets. Hence the only matrix element we need to consider connects the $\ell_{14} = \ell_{23} = 1, j = 0$ ground state to the $\ell_{14} = \ell_{23} = j = 1$ first excited state. The strength/site of this response is $2/3$. No other states are excited. Identical results are found, of course, for larger systems in the limit of non-interacting plaquettes. Exact calculations of this response for $2 \times L$ ladders with $L = 2, 4, 6$ and 8 are remarkably consistent with this simple picture; a large fraction—typically in excess of 96%—of the total $S(\vec{q}_{\pi\pi}, \omega)$ strength is concentrated in the lowest triplet level. The response/site to this level grows slowly but steadily from a value of $2/3$ for $L = 2$ to 0.99934 for $L = 8$. We again emphasize the role of the plaquette basis in understanding the basic features of $S(\vec{q}_{\pi\pi}, \omega)$.

Because the $\vec{S}(\vec{q}_{\pi\pi})$ operator cannot connect states in the frozen basis to outside states, a high-quality description of $S(\vec{q}_{\pi\pi}, \omega)$ utilizing the frozen basis should be possible. Moreover, CORE prescribes how any operator—not just the Hamiltonian—should be renormalized to account for truncations. We here present calculations of $S(\vec{q}_{\pi\pi}, \omega)$ in the frozen basis including range-3 renormalization corrections for both the Hamiltonian and the transition operator for $2 \times L$ systems with $L = 6, L = 8$, and 16 . For $L = 6$ a range-3 calculation is exact—at least for the low-energy part of the response (see Fig.1). For $L = 8$ a range-3 CORE calculation is no longer exact but we can compare with exact results. We find that the range-3 CORE calculation for the integrated response to the lowest triplet level, $S(\vec{q}_{\pi\pi}, \Delta) \equiv |\langle \Psi_{n=1} | \vec{S}(\vec{q}) | \Psi_0 \rangle|^2$, differs from the exact value by less than 0.014%. All our calculations of $S(\vec{q}_{\pi\pi}, \Delta)$ are summarized in Table I and in Figure 2. There we see that the range-3 renormalization corrections to the spin operator [Eq. (8)] tend to reduce $S(\vec{q}_{\pi\pi}, \Delta)$; this is true of all induced CORE contributions and we therefore assume that the CORE results for the 2×16 ladder are upper limits. Based on the accuracy of CORE for 2×8 ladders, we speculate that the error in our 2×16 result is less than 0.1%.

The following picture of $S(\vec{q}_{\pi\pi}, \omega)$ emerges from our calculations. As the length of the ladder grows from $L = 2$, the great majority of strength remains concentrated in the lowest triplet state. At the same time, moderately strong coherent many-body effects increase the response/site to the first triplet state from $2/3$ for the smallest system for which this response can be defined, namely, a single 2×2 plaquette, to a value of 1.088 for $L = 16$. Extrapolation to the thermodynamic limit is somewhat ambiguous but we speculate that, in this limit, $S(\vec{q}_{\pi\pi}, \Delta)/\text{site}$ will lie between 1.10 and 1.12 —which corresponds to an enhancement over the single-plaquette value by a factor of around 1.6 . It would be very interesting to see the extent to which these predictions are consistent with, *e.g.*, future neutron scattering measurements utilizing single-crystal ladder compounds.

In summary, we have used the recently proposed plaquette basis [8] to investigate static and dynamic properties of isotropic 2-leg Heisenberg spin ladders. This basis reveals some of the important physics of these complicated systems in an especially clear fashion. For example, we find that the low-energy states of these ladders are dominated by the relatively few configurations in which the diagonal spins of the plaquettes are frozen in triplets. This means that an extreme truncation of the basis which retains only the frozen states will nevertheless be reasonably accurate. When truncation errors are corrected for using the recently developed CORE approach [11], we are able to compute properties of 2×16 ladders with great precision. In addition to static quantities such as the energy/site and the gap, we are also able to calculate the dynamical spin response $S(\vec{q}_{\pi\pi}, \omega)$. As the operator which

governs this response cannot break the frozen spin triplets, accurate calculations of $S(\vec{q}_{\pi\pi}, \omega)$ are possible in the truncated basis and these, too, can be systematically improved via the CORE technology. Moreover, just as a simple picture of non-interacting multi-plaquette states gives a surprisingly accurate estimate of the energy/site of large systems, the same picture also tells us a great deal about $S(\vec{q}_{\pi\pi}, \omega)$. Specifically, we see that the bulk of the response is concentrated in the lowest triplet state and that the response/site is of order 1.

We emphasize the computational efficiencies achievable when using CORE with the truncated plaquette basis. Because the bulk of the $S(\vec{q}_{\pi\pi}, \omega)$ response lies in the lowest triplet excitation and we can focus on this single transition, still greater efficiencies are possible. Specifically we may use a simple 2×2 Lanczos technique [14] to find only the lowest eigenvalue and eigenvector in the singlet and triplet sectors rather than performing the much more time-consuming full diagonalizations. With these efficiencies, calculation of the 2×16 response $S(\vec{q}_{\pi\pi}, \Delta)$ presented here required only 12 minutes of CPU time on a PC. In addition to providing new results for the dynamic spin response—which we hope can soon be compared with new data for inelastic neutron scattering from single crystals of ladder compounds—we have demonstrated the utility of the plaquette basis both for numerical studies and for illuminating the important physics of spin ladders.

ACKNOWLEDGMENTS

We thank E. Dagotto, M. Laukamp, F.X. Lee, and G.B. Martins for many useful and stimulating discussions. This work was supported by the DOE under Contracts Nos. DE-FC05-85ER250000, DE-FG05-92ER40750 and DE-FG03-93ER40774.

REFERENCES

- [1] E. Dagotto and T.M. Rice, *Science* **271**, 618 (1996).
- [2] E. Dagotto, J. Riera and D.J. Scalapino, *Phys. Rev. B* **45**, 5744 (1992).
- [3] D.C. Johnston, J.W. Johnson, D.P. Gorshorn and A.P. Jacobson, *Phys. Rev. B* **35**, 219 (1987).
- [4] T. Barnes, E. Dagotto, J. Riera and E.S. Swanson, *Phys. Rev. B* **47**, 3196 (1993).
- [5] S.R. White, R.M. Noack and D.J. Scalapino, *Phys. Rev. Lett.* **73**, 886 (1994).
- [6] S. Sachdev and R.N. Bhatt, *Phys. Rev. B* **41**, 9323 (1990).
- [7] M. Sigrist, T.M. Rice, F.C. Zhang, *Phys. Rev. B* **49**, 12058 (1994).
- [8] J. Piekarewicz and J.R. Shepard, *Phys. Rev. B*, in press.
- [9] E. Dagotto, G.B. Martins, J. Piekarewicz, J. Riera, and J.R. Shepard, preprint.
- [10] See, *e.g.*, D.M. Brink and G.R. Satchler, *Angular Momentum*, Clarendon Press (Oxford) 1993.
- [11] C.J. Morningstar and M. Weinstein, *Phys. Rev. Lett.* **73**, 1873 (1994); *Phys. Rev. D* **54**, 4131 (1996).
- [12] Markus Laukamp, private communication.
- [13] R.S. Eccleston, T. Barnes, J. Brody and J.W. Johnson, *Phys. Rev. Lett.* **73**, 2626 (1994).
- [14] E. Dagotto and A. Moreo, *Phys. Rev. D* **21**, 865 (1985); E. Gagliano, E. Dagotto, A. Moreo, and F. Alcaraz, *Phys. Rev. B* **34**, 1677 (1986).

FIGURES

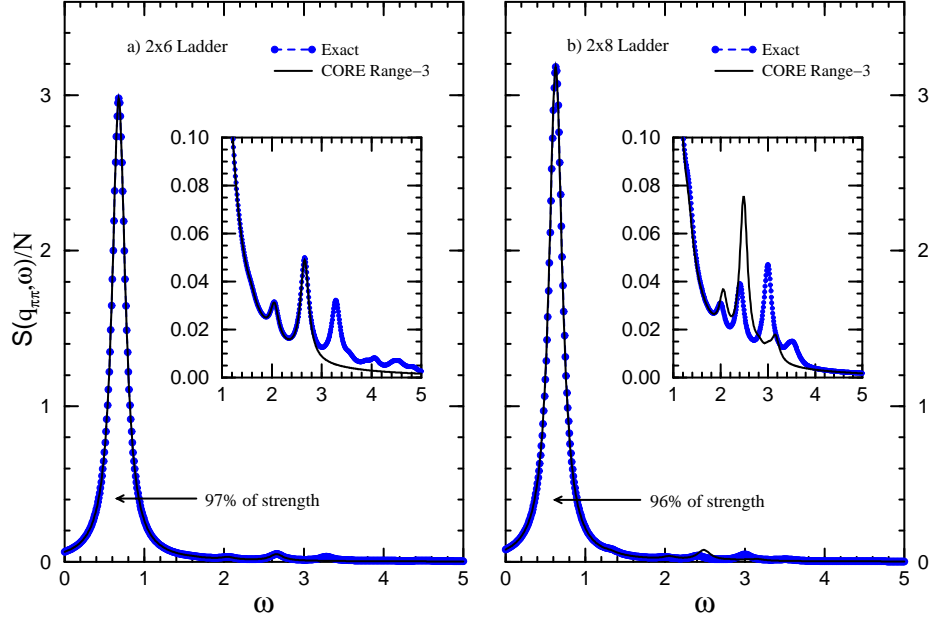


FIG. 1. Dynamic spin response for a) 2×6 and b) 2×8 ladders; an artificial width of 0.1 is included.

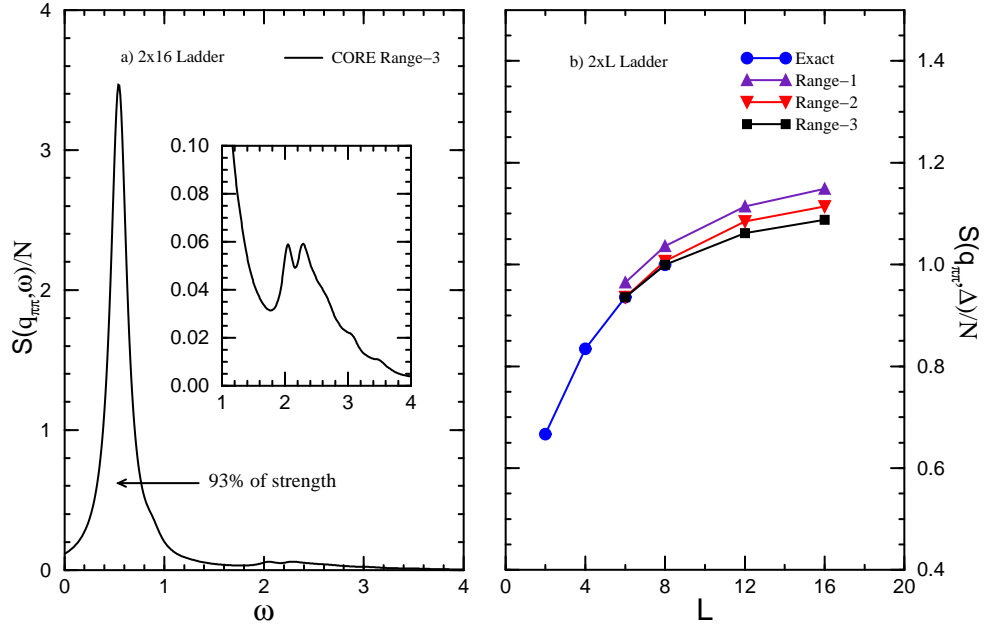


FIG. 2. Dynamic spin response a) for a 2×16 ladder; an artificial width of 0.1 is included and b) to the lowest triplet state as a function of the length of the ladder.

TABLES

TABLE I. Static and dynamical properties of a 2×8 (first set of numbers) and a 2×16 (last set of numbers) Heisenberg ladder. Quantities in parenthesis represent the discrepancy with the exact or DMRG values, respectively.

Observable	CORE range-3	Exact	CORE range-3	DMRG
E_0/site	$-0.55711(0.020\%)$	-0.55722	$-0.56742(0.037\%)$	-0.56763
E_1/site	$-0.51784(0.012\%)$	-0.51778	$-0.55041(0.018\%)$	-0.55031
$E_1 - E_0$	$0.62835(0.423\%)$	0.63101	$0.54441(1.782\%)$	0.55411
$S(\vec{q}_{\pi\pi}, \Delta)/\text{site}$	$0.99920(0.014\%)$	0.99934	1.08785	NA